Supporting Information

A collection of topological types of nanoclusters and its application to icosahedron-based intermetallics

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Table S1. The graphs of most abundant 0@12 and 1@12 nanocluster configurations and their occurrences in intermetallics.

0@12 graphs are subgraphs of the corresponding centered 1@12 graphs and always occur in all structures, where the 1@12 graph exists. For example, the 3543 1@*ico* structures contain also the 0@*ico* graph as a subgraph of 1@*ico*. Other 3600 – 3543 = 57 structures contain only 0@*ico* graphs, not 1@*ico*.

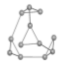
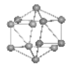
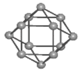
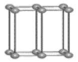
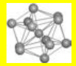
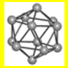
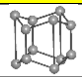
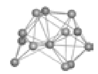
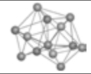
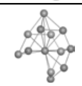
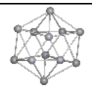
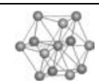
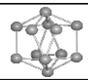
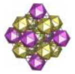
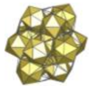
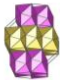
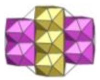
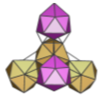
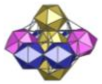
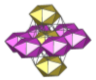
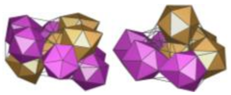
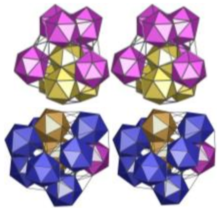
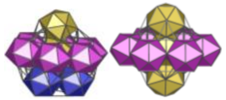
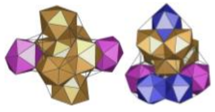
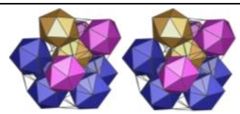
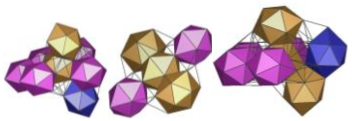
Nanocluster Symbol	Occurrence	Graph	Nanocluster Symbol	Occurrence	Graph
0@12_model1	27963		1@12_model24	6147	
0@12_model3	27760		1@12_model64	5892	
0@12_model5	25922		1@12_model68	4679	
0@12_model9	7827		1@12_model65	3945	
0@12_model8	6316		1@12_model42	3830	
0@12_model2	4313		1@12_model1 (*1@ico*)	3543	
0@12_model12 (*0@ico*)	3600		1@12_model25	3359	
0@12_model4	2739		1@12_model8	3123	
0@12_model13	2086		1@12_model6	2579	
0@12_model10	1263		1@12_model66	2290	
0@12_model11	585		1@12_model5	2102	
0@12_model6	23		1@12_model28	2078	
0@12_model14	9		1@12_model2	1413	
0@12_model7	2		59 more models	1344-1	…

Table S2. Distribution of local binding of icosahedra in the 1506 intermetallics assembled with one non-equivalent icosahedron

Formula		**Underlying net**	**Topological types**	**Number of structures**	**Formula**		**Underlying net**	**Topological types**	**Number of structures**
$1@ico^{8+6}_{f_3^1+e^1}$		**bcu-x**	Mo_3Zr	**427**	$1@ico^{2+6}_{f_3^1+b^4}$		**hex**	Co_2Al_5	**2**
$1@ico^{8+6}_{b^6+b^2}$		**bcu-x**	WAl_{12}	**9**	$1@ico^{3+4}_{e^1+v^1}$		**($3^6.4^{12}.5^3$)***	$NdTi_3(Sn_{0.1}Sb_{0.9})_4$	**2**
$1@ico^{2+8+4}_{e^1+b^4+b^1}$		**bcu-x**	$Nb(Cu_{0.5}Ga_{0.5})$	**1**	$1@ico^{6}_{f_3^1}$		**crs**	Ti_2Ni, Gd_4RhIn	**100**
$1@ico^{12}_{v^1}$		**fcu**	$CeRu_2Mg_5$	**1**	$1@ico^{6}_{f_3^1}$		**pcu**	Ca_3Ag_8	**19**
$1@ico^{6+6}_{f_3^2+e^1}$		**fcu**	Cu_2GaSr $SrNi_2Ge$ $BaNi_2Ge$	**4**	$1@ico^{6}_{f_3^2}$		**hxl***	Sr_2Ni_3	**1**
$1@ico^{6+6}_{f_3^1+v^1}$		**fcu**	$AlAu_4$	**9**	$1@ico^{4+2}_{v^1+e^1}$		**hxl***	Yb_2Ag_7 Hf_2Co_7 Zr_2Ni_7	**4**
$1@ico^{1+3+6}_{f_3^1+v^1+e^1}$		**tca**	$TaCo_2$	**81**	$1@ico^{4+2}_{f_3^1+e^1}$		**hxl***	$Al_{2.88}Ta_{2.66}V_{1.46}$	**1**
$1@ico^{3+6}_{f_3^1+v^1}$		**ncb**	Ni_4Zn_{22} Cu_5Zn_8	**22**	$1@ico^{2+4}_{f_3^2+e^1}$		**hxl***	$Sr_2Rh_2In_3$	**1**
$1@ico^{2+6}_{f_3^1+e^1}$		**hex**	WBe_2 Fe_2Ta	**766**	$1@ico^{2+2}_{e^1+b^7}$		**dia**	$Fe_2Ga_6Sc_3$, Hf_3Cu_8	**5**
$1@ico^{2+2+4}_{f_3^1+e^1+v^1}$		**hex**	$PuCu_6$	**39**	$1@ico^{2+2}_{f_3^1+e^1}$		**sql***	Cs_3NaPb_4	**1**
$1@ico^{2+6}_{b^{12}+e^1}$		**hex**	K_2Hg_7	**2**	$0@ico^{6}_{f_3^1}$		**lcy**	$Y_5Ag_3Cu_{12}$	**1**
$0@ico^{2+8+4}_{e^1+b^4+b^1}$		**bcu-x**	Nb_2Al	**1**	$0@ico^{2+6}_{f_3^1+e^1}$		**hex**	WBe_2	**7**

* – ignoring bonds between icosahedra that unite layers into a 3D framework.

Table S3. Distribution of local binding of icosahedra in the 22 intermetallics assembled with two or three non-equivalent icosahedra

Formula		**Underlying net**	**Topological types**	**Number of structures**
$2(1@ico^{3+6}_{f_3^1+v^1})$		**ncb**	Mn_3In, $Ag_9Ca_8Hg_9$, $Cd_{43}Pd_8$	**8**
$2(1@ico^{1+6+3}_{f_3^1+e^1+v^1}) + 1@ico^{2+6}_{f_3^1+e^1}$		$\mathbf{(3^{15}.4^{24}.5^{6})_2(3^{6}.4^{18}.5^{3}.6)}$	(AlCu)Mg	**3**
$1@ico^{3+6}_{f_3^1+e^1} + 1@ico^{3+4}_{f_3^1+e^1}$		$\mathbf{(3^{13}.4^{14}.5^{9})(3^{8}.4^{8}.5^{5})}$	$(Cr_9Mo_{21}Ni_{20})_{1.12}$	**3**
$2(1@ico^{3+6}_{f_3^1+v^1})$ $2(1@ico^{1+1+9}_{f_3^1+e^1+v^1})$		$\mathbf{(3^{12}.4^{12}.5^{12})(3^{12}.4^{14}.5^{10})}$ $\mathbf{(3^{18}.4^{28}.5^{9})}$	MoNi	**1**
$1@ico^{1+3+6}_{f_3^1+v^1+e^1} + 1@ico^{2+6}_{f_3^1+e^1}$		$\mathbf{(3^{15}.4^{24}.5^{6})(3^{6}.4^{18}.5^{3}.6)}$	$Mg_{16}Zn_{31}Cu$	**1**
$1@ico^{6+2}_{f_3^1+v^1} + 1@ico^{4+2+4}_{f_3^1+e^1+v^1}$		$\mathbf{(3^{10}.4^{12}.5^{6})(3^{11}.4^{16}.5^{18})}$	$HfCrGa_2$	**3**
$2(1@ico^{4+2+4}_{f_3^1+e^1+v^1})$		$\mathbf{(3^{13}.4^{21}.5^{11})(3^{17}.4^{21}.5^{7})}$	$Y_2Ni_7Sn_3$	**1**
$2(1@ico^{1+3+5}_{f_3^1+e^1+v^1})$		$\mathbf{(3^{12}.4^{19}.5^{5})(3^{9}.4^{19}.5^{8})}$	$Al_7Nb_{24}Ni_{21}$	**1**
$1@ico^{1+5+1}_{f_3^1+e^1+v^1} + 1@ico^{2+2}_{f_3^1+e^1} + 1@ico^{2+4+1}_{f_3^1+e^1+v^1}$		$\mathbf{(3^{4}.4^{8}.5^{7}.6^{2})_2(3^{5}.4^{9}.5^{7})_2(4^{4}.6^{2})}$	$Nb_{28}Ni_{33.56}Sb_{12.44}$	**122**

* – ignoring bonds between icosahedra that unite layers into a 3D framework.

Table S4. Chemical composition of 324 binary intermetallics assembled with one non-equivalent icosahedron

Space group	Point group	Supracluster	Underlying net	Central atom (A)	Environment (M)	Structure topology	Number of structures
I m$\bar{3}$m	$\bar{3}m$	$1@ico^{6}_{f_3^1}$	pcu	Ag	A_6+M_6 (M = Ca)	**12,12,16T1**	1
F d$\bar{3}$m	$\bar{3}m$	$1@ico^{6}_{f_3^1}$	crs/dia-e	Co	A_6+M_6 (M = Hf)	**12,12,14T1**	27
				Hf	A_6+M_6 (M = Fe, Ir, Mn, Os, Pd, Pt, Rh)		
				Mg	A_6+M_6 (M = Pd)		
				Mn	A_6+M_6 (M = Hf)		
				Na	A_6+M_6 (M = Ba)		
				Ni	A_6+M_6 (M = Cd); M12 (M=Nb, Ta)		
				Sc	A_6+M_6 (M = Ni, Pd, Ir)		
				Ti	A_6+M_6 (M = Co, Cu, Fe, Ni)		
				Zr	A_6+M_6 (M = Cu, Co, Ir, Pt, Rh, Fe)		
P m$\bar{3}$n	$m\bar{3}$	$1@ico^{8+6}_{f_3^1+e^1}$	bcu-x	Al	M_{12} (M = Mo, Nb, V)	**bet**	78
				Au	M_{12} (M = Ta, Zr, Ti, V, Nb, Ti)		
				Be	M_{12} (M = Mo)		
				Bi, Sn	M_{12} (M = Nb)		
				Cd, Co, Fe, Ni	M_{12} (M = V)		
				Ga, Ge	M_{12} (M = Cr, Mo, Nb, V)		
				Hg	M_{12} (M = Ti, Zr)		
				In	M_{12} (M = Nb)		
				Ir, Pt	M_{12} (M = V, Cr, Ti, Mo, Nb)		
				Os	M_{12} (M = Cr, Mo, Nb)		
				Pb	M_{12} (M = Nb, V)		
				Pd	M_{12} (M = Ti)		
				Re	M_{12} (M = W)		
				Rh	M_{12} (M = Cr, Nb, V)		
				Ru	M_{12} (M = Cr)		
				Sb	M_{12} (M = Nb, Ta, Ti, V)		
				Sn	M_{12} (M = Mo, Nb, Zr, Ta, V)		
				Tl	M_{12} (M = Nb)		
				V	M_{12} (M = Ge, Re, Sb)		
				Zr	M_{12} (M = Mo)		
I $\bar{4}$3m	$3m$	$1@ico^{3+6}_{f_3^1+v^1}$	ncb	Ni, Rh, Ir	M_{12} (M = Zn)	**12,12,13,13T1**	5
				Cu	A_3 + M_9 (M = Zn		
				Ag	A_3 + M_9 (M = Cd)		
I m$\bar{3}$	$m\bar{3}$	$1@ico^{8+6}_{b^6+b^2}$	bcu-x	Mo, Re, Tc, W	M_{12} (M = Al)	**11,12T1**	5
P $2_1$3	3	$1@ico^{6+6}_{f_3^2+e^1}$	fcu	Al	M_{12} (M = Au, Cu)	**12,14T1**	2
				Au	A_9+M_3 (M = Al)		
				Cu	A_9+M_3 (M = Al)		
P 6_3/mmc	$3m$	$1@ico^{1+3+6}_{f_3^1+v^1+e^1}$	tca	Al	A_6+M_6 (M = U)	**12,12,12,16,16T1**	21
				Co	A_6+M_6 (M = Nb, Ta, Ti)		
				Cr	A_6+M_6 (M = Ti, Hf, Zr)		
				Fe	A_6+M_6 (M = Nb, Hf, Sc, Zr)		
				Mg	A_6+M_6 (M = Th)		
				Mn	A_6+M_6 (M = Zr, Hf)		
				Mo	A_6+M_6 (M = Hf)		
				Ni	A_6+M_6 (M = Eu, Mg)		
				Zn	A_6+M_6 (M = Hf, Nb, Ta)		

Table S4 continuation

	$\bar{3}m$	$1@ico^{2+6}_{f_3^1+e^1}$	hex	Ag, Au Al Be Cd Co Cr Cu Fe Ir K Li, Pt Mg Mn Na Ni Os Pb Re Ru Tc V Zn	A_6+M_6 (M = K) A_6+M_6 (M = Hf, Zr, Co) A_6+M_6 (M = Cr, Fe, Mn, Mo, Ru, V, W, Re) A_6+M_6 (M = Ca, Yb) A_6+M_6 (M = Ta, Nb, Mg) A_6+M_6 (M = Nb, Hf, Ta, Ti, Zr) A_6+M_6 (M = Cd, Yb) A_6+M_6 (M = Er, Eu, Ho, Lu, Mo, Tb, Tm, Yb, Hf, Nb, Sc, Ti, W, Ta) A_6+M_6 (M = Mg) A_6+M_6 (M = Cs) A_6+M_6 (M = Ca) A_6+M_6 (M = Ba, Ca, Dy, Er, Eu, Ho, Lu, Sr, Tb, Tm, Y, Yb) A_6+M_6 (M = Dy, Er, Gd, Hf, Ho, Lu, Pr, Ta, Tm, Tb, Y, Nd, Yb, Sc, Sm, Th, Zr) A_6+M_6 (M = Ba, Cs, K) A_6+M_6 (M = Nb, U) A_6+M_6 (M = Am, Dy, Er, Gd, Hf, Ho, La, Lu, Nd, Tb, Tm, U, Yb, Pr, Pu, Sc, Sm, Y, Zr) A_6+M_6 (M = K) A_6+M_6 (M = Dy, Er, Eu, Gd, Hf, Ho, Nd, Np, Pr, Pu, Sm, Tb, Th, Tm, U, W, Y, Sc, Zr) A_6+M_6 (M = Dy, Er, Ho, Lu, Nd, Sm, Tb, Tm, Yb, Sc, Y, Zr) A_6+M_6 (M = Dy, Er, Gd, Hf, Ho, Tc, Tb, Th, Tm, Y, Zr) A_6+M_6 (M = Zr) A_6+M_6 (M = Ca, Mg, Sc, Sr, Ta, Ti)	**mgz-x**	153
		$1@ico^{2+6}_{f_3^1+b^4}$	hex	Al	A_6+M_6 (M = Cu, Rh)	**3-nodal net; 9,12,12-coordinated**	2
P 6_3mc	*3m*	$1@ico^{2+6}_{f_3^1+e^1}$	hex	Mn	A_9+M_3 (M = Lu)	**mgz-x**	1
P $\bar{3}$m1	$\bar{3}m$	$1@ico^{2+6}_{b^{12}+e^1}$	hex	Hg	A_6+M_6 (M = K, Rb)	**11,12,18T2**	2
P 4_2/mmc	*mmm*	$1@ico^{8+6}_{f_3^1+e^1}$	bcu-x	Sn	M_{12} (M = Nb)	**bet**	1
C mcm	*m2m*	$1@ico^{2+6}_{f_3^1+e^1}$	hex	Re	A_6+M_6 (M = U)	**mgz-x**	1
	mm2	$1@ico^{4+2}_{v^1+e^1}$	hxl	Ag	A_8+M_4 (M = Ca, Yb)	**12,12,12,16T1**	2
P nma	*m*	$1@ico^{2+2+4}_{f_3^1+e^1+v^1}$	hex	Cu	A_9+M_3 (M = Ce, La, Pr, Pu, Sm, Th, Nd)	**12,12,12,13,14,19T1**	7
		$1@ico^{2+2}_{e^1+b^7}$	dia	Cu	A_9+M_3 (M = Hf) A_7+M_5 (M = Zr)	**11,12,12,12,12,13,13,14T1**	2
P 2_1/c	*1*	$1@ico^{2+2+4}_{f_3^1+e^1+v^1}$	hex	Cu	A_9+M_3 (M = Ce, La, Pr, Nd)	**12,12,12,13,14,19T1**	4
C 2/m	*m*	$1@ico^{4+2}_{v^1+e^1}$	hxl	Co Ni	A_8+M_4 (M = Hf) A_8+M_4 (M = Zr)	**6-nodal net; 12,12,12,13,15,16-coordinated**	2

P 6_3/mmc	$\bar{3}m$	$0@ico^{2+6}_{f_3^1+e^1}$	hex	0	M^1_6+M^2_6 (M^1 = Al, M^2 = Er, Lu, U) M^1_6+M^2_6 (M^1 = Co, M^2 = U) $M1_6$+M^2_6 (M^1 = Be, M^2 = V, W)	**2-nodal net; 10,13-coordinated**	7
P 4_2/mnm	*mmm*	$0@ico^{2+8+4}_{e^1+b^4+b^1}$	bcu-x	0	M^1_8+M^2_4 (M^1 = Nb, M^2 = Al)	**3-nodal net; 8,9,11-coordinated**	1

* – ignoring bonds between icosahedra that unite layers into a 3D framework.

Table S5. Chemical composition of 90 ternary intermetallics constructed by one nonequivalent icosahedron

Space group	Point group	Supracluster	Underlying net	Central atom (A)	Environment (M)	Structure topology	Number of structures
I $m\bar{3}m$	$\bar{3}m$	$1@I^{6}_{f_3^1}$	pcu	Al	$M^1_6+M^2_6$ (M^1 = Ni, M^2 = Y, Sm, Gd, Dy, Ho, Er, Tb)	12,12,16T1	17
				Ga	$M^1_6+M^2_6$ (M^1 = Ni, M^2 = Y, Sm, Gd, Dy, Ho, Er, Tb, Tm, Pr, Nd)		
F $d\bar{3}m$	$\bar{3}m$	$1@I^{6}_{f_3^1}$	crs/dia-e	Ag	$M^1_6+M^2_6$ (M^1 = Na, M2 = In)	12,12,14T1	12
				Al	$M^1_6+M^2_6$ (M^1 = Mg, Hf, Zr, M^2 = Ni, Au, Pt)		
				Au	$M^1_6+M^2_6$ (M^1 = Na, M^2 = In)		
				Ge	$M^1_6+M^2_6$ (M^1 = Ni, M^2 = Zn)		
				Mn	$M^1_6+M^2_6$ (M^1 = Mg, M^2 = Ni)		
				Ti	$M^1_6+M^2_6$ (M^1 = Mg, M^2 = Ni)		
				Zn	$M^1_6+M^2_6$ (M^1 = Cu, M^2 = Hf, Zr)		
F $\bar{4}3m$	*3m*	$1@I^{6}_{f_3^1}$	crs/dia-e	Dy	$A_6+M^1_3+M^2_3$ (M^1 = Cd, In, M^2 = Rh)	9,12,12,14,14T1	17
				Er	$A_6+M^1_3+M^2_3$ (M^1 = In, M^2 = Rh, Ir)		
				Gd	$A_6+M^1_3+M^2_3$ (M^1 = Cd, In, M^2 = Rh, Ni, Pd, Ir, Pt)		
				Ho	$A_6+M^1_3+M^2_3$ (M^1 = Cd, In, M^2 = Rh, Ir, Pt)		
				Tm	$A_6+M^1_3+M^2_3$ (M^1 = In, M^2 = Rh)		
				Tb	$A_6+M^1_3+M^2_3$ (M^1 = In, Cd, M^2 = Ir, Rh)		
P 2_13	*3*	$1@I^{6+6}_{f_3^1+v^1}$	fcu	Au	$M^1_9+M^2_3$ (M^1 = Cu, Nb, Ta, V, M^2 = Sn, Ga)	12,14T1	5
				Ga	$M^1_9+M^2_3$ (M^1 = Nb, Ta, V, M^2 = Au)		
				Ge	$M^1_9+M^2_3$ (M^1 = Mn, M^2 = Ir)		
				Ir	$M^1_9+M^2_3$ (M^1 = Mn, M^2 =Ge)		
				Sn	$M^1_9+M^2_3$ (M^1 = Cu, M^2 = Au)		
P $6_3/mmc$	$\bar{3}m$	$1@I^{2+6}_{f_3^1+e^1}$	hex	Al	$M^1_6+M^2_6$ (M^1 = Co, M^2 = U)	mgz-x	18
				Co	$M^1_6+M^2_6$ (M^1 = Al, M^2 = Lu, Er)		
				Ga	$M^1_6+M^2_6$ (M^1 = Fe, M^2 = U, Zr)		
				Ge	$M^1_6+M^2_6$ (M^1 = Mn, Ti, Fe, Co, M^2 = Co, Zr, U, Cu)		
				Ir	$M^1_6+M^2_6$ (M^1 = Ga, M^2 = Eu)		
				Os	$M^1_6+M^2_6$ (M^1 = Al, M^2 = U)		
				Ru	$M^1_6+M^2_6$ (M^1 = Al, V, M^2 = Sc, Zr)		
				Li	$M^1_6+M^2_6$ (M^1 = Na, M^2 = Au)		
				Ge	$M^1_6+M^2_6$ (M^1 = V, M^2 = Hf)	12,12,15T2	1
		$1@I^{6+2}_{f_3^2+f_3^1}$		Ge	$M^1_6+M^2_6$ (M^1 = Ni, M^2 = Sr)	10,12,20T1	1
P 6_3mc	*3m*	$1@I^{2+6}_{f_3^1+e^1}$	hex	Cu	$A_6+M^1_3+M^2_3$ (M^1 = Mn, M^2 = In)	mgz-x	1
R $\bar{3}m$	$\bar{3}m$	$1@I^{6+6}_{f_3^2+e^1}$	fcu	Ga	$M^1_6+M^2_6$ (M^1 = Cu, M^2 = Sr, Ba)	10,12,20T2	2
P *42/ncm*	*2/m*	$1@I^{12}_{v^1}$	fcu	Mg	$A_8+M^1_2+M^2_2$ (M^1 = Ru, M^2 = Ce)	10,12,15,16T1	1
C *mcm*	*2/m*	$1@I^{2+6}_{f_3^1+e^1}$	hex	Ga	$A_4+M^1_6+M^2_2$ (M^1 = Mg, M^2 = Mn)	mgz-x	1
C *mcm*	*2/m*	$1@I^{2+2}_{f_3^1+e^1}$	sql	Na	$M^1_6+M^2_6$ (M^1 = Cs, M^2 = Pb)	10,12,12,14,18T1	1
P *nma*	*m*	$1@I^{2+2}_{e^1+b^7}$	dia	Fe	$A_3+M^1_5+M^2_4$ (M^1 = Zr, M^2 = Sn)	11,12,12,12,12,13,13,14T1	1
				Fe	$A+M^1_5+M^2_6$ (M^1 = Sc, M^2 = Ga)	11,12,12,12,12,13,16,17T1	2
				Mn	$A+M^1_5+M^2_6$ (M^1 = Sc, M^2 = Ga)		
		$1@I^{2+2+4}_{f_3^1+e^1+v^1}$	hex	Cu	$A_7+M^1_2+M^2_3$ (M^1 = In, Sn, Ag, Au, M^2 = Ce, U, Th)	12,12,12,13,14,19T1	8
				Fe	$A_7+M^1_2+M^2_3$ (M^1 = Sn, M^2 = U)		
				Ni	$A_7+M^1_2+M^2_3$ (M^1 = Sn, M^2 = Lu)		
P *mmn*	*mm2*	$1@I^{6}_{f_3^2}$	hxl	Ge	$M^1_6+M^2_6$ (M^1 = Ni, M^2 = Ba)	10,12,20T3	1
C *2/m*	*2/m*	$1@I^{2+4}_{f_3^2+e^1}$	hxl	In	$A_2+M^1_4+M^2_6$ (M^1 = Rh, M^2 = Sr)	10,12,12,17T1	1

* – ignoring bonds between icosahedra that unite layers into a 3D framework.

Table S6. Central atoms and environment atoms in the centered icosahedra

Central atom (A)	Environment (M)
Ag	Ag, Ca, Cd, K, Yb, Na, In
Al	Al, Mo, Nb, V, Au, Cu, U, Hf, Zr, Co, Rh, Ni, Y, Sm, Gd, Dy, Ho, Er, Tb, Mg, Pt
Au	Au, Ta, Zr, Ti, V, Nb, Al, K, Na, In, Cu, Sn, Ga
Be	Be, Mo, Cr, Fe, Mn, Ru, V, W, Re
Bi	Nb
Cd	Cd, V, Ca, Yb
Co	Co, Hf, V, Nb, Ta, Ti, Mg, Al, Lu, Er
Cr	Cr, Ti, Hf, Zr, Nb, Ta
Cu	Cu, Al, Cd, Yb, Ce, La, Pr, Pu, Sm, Th, Nd, Hf, Zr, Mn, In, Sn, Ag, Au, U, Zn
Dy	Dy, Cd, In, Rh
Er	Er, In, Rh, Ir
Fe	Fe, V, Nb, Hf, Sc, Zr, Er, Eu, Ho, Lu, Mo, Tb, Tm, Yb, Ti, W, Ta, Sn, Ga, U
Ga	Ga, Cr, Mo, Nb, V, Ni, Y, Sm, Gd, Dy, Ho, Er, Tb, Tm, Pr, Nd, Ta, Au, Fe, U, Zr, Cu, Sr, Ba, Mg, Mn
Gd	Gd, Cd, In, Rh, Ni, Pd, Ir, Pt
Ge	Cr, Mo, Nb, V, Ni, Zn, Mn, Ir, Ti, Fe, Co, Zr, U, Cu, Hf, Sr, Ba
Hf	Hf, Fe, Ir, Mn, Os, Pd, Pt, Rh
Hg	Hg, Ti, Zr, K, Rb
Ho	Ho, Cd, In, Rh, Ir, Pt
In	In, Nb, Rh, Sr
Ir	Ir, V, Cr, Ti, Mo, Nb, Mg, Mn, Ge, Ga, Eu, Zn
K	K, Cs
Li	Li, Ca, Na, Au
Mg	Mg, Pd, Th, Ba, Ca, Dy, Er, Eu, Ho, Lu, Sr, Tb, Tm, Y, Yb, Cu, Ru, Ce
Mn	Mn, Hf, Zr, Dy, Er, Gd, Ho, Lu, Pr, Ta, Tm, Tb, Yb, Nd, Sc, Sm, Th, Cu, Rh, Mg, Ni, Ga, In, Ti, Al, Nb, Y
Mo	Mo, Al, Hf
Na	Na, Ba, Cs, K, Pb
Ni	Ni, Cd, Nb, Ta, V, Zn, Eu, Mg, U, Zr, Sn, Lu
Os	Os, Cr, Mo, Nb, Am, Dy, Er, Gd, Hf, Ho, La, Lu, Nd, Tb, Tm, U, Yb, Pr, Pu, Sc, Sm, Zr, Al
Pb	Pb, Nb, V, K
Pd	Ti
Pt	Pt, V, Cr, Ti, Mo, Nb, Ca
Re	Re, W, Al, Dy, Er, Eu, Gd, Hf, Ho, Nd, Np, Pr, Pu, Sm, Tb, Th, Tm, U, Y, Sc, Zr, Y
Rh	Cr, Nb, V, Zn
Ru	Ru, Cr, Dy, Er, Ho, Lu, Nd, Sm, Tb, Tm, Yb, Sc, Y, Zr, Al, V
Sb	Nb, Ta, Ti, V
Sc	Sc, Ni, Pd, Ir
Sn	Nb, Mo, Zr, Ta, V, Cu, Au
Tb	Tb, In, Cd, Ir, Rh
Tc	Tc, Al, Dy, Er, Gd, Hf, Ho, Tb, Th, Tm, Y, Zr
Ti	Ti, Co, Cu, Fe, Ni, Mg
Tl	Nb
Tm	Tm, In, Rh
V	V, Ge, Re, Sb, Zr
W	Al
Zn	Zn, Nb, Hf, Ta, Ca, Mg, Sc, Sr, Ti, Cu, Zr
Zr	Zr, Cu, Co, Ir, Pt, Rh, Fe, Mo

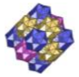
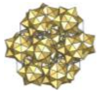
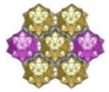
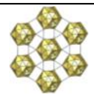
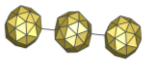
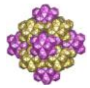
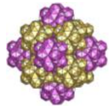
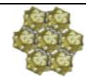
Table S7. Central atoms and environment atoms in the centered icosahedra with a mixed M^1+M^2 shell.

Environment A/M^1	**Environment M^2**
Li	Ca
Be	Cr, Fe, Mn, Mo, Ru, V, W, Re
Na	Ba, Cs, K, In, Au
Mg	Co, Ir, Pd, Th, Ba, Ca, Dy, Er, Eu, Ho, Lu, Sr, Tb, Tm, Yb, Ni, Pt, Ru, Ce, Mn, Zn, Y
Al	U, Hf, Zr, Co, Cu, Rh, Lu, Er, Sc, Er, Au, Nb
K	Ag, Au, Hg, Na, Pb
Ca	Ag, Cd, Li, Mg, Pt, Zn
Sc	Al, Fe, Mn, Os, Re, Ru, Ni, Pd, Ir, Ga, Zn
Ti	Co, Cr, Fe, Co, Cu, Fe, Ni, Zn
V	Zr, Hf
Cr	Ti, Hf, Zr, Nb, Ta
Mn	Cu, Ga, Hf, Mg, Zr, Dy, Er, Gd, Ho, Lu, Pr, Ta, Tm, Tb, Yb, Nd, Sc, Sm, Th, Ir, Ge, U, Co, In, Y
Fe	Nb, Hf, Sc, Zr, Er, Eu, Ho, Lu, Mo, Tb, Yb, Ti, W, Ta, U, Sn, Ga
Co	Al, Hf, Nb, Ta, Ti, Mg, U, Mn, Zr
Ni	Cd, Gd, Mg, Eu, Nb, U, Zr, Y, Sm, Dy, Ho, Er, Tb, Tm, Pr, Nd, Zn, Sr, Ba, Sc, Ti
Cu	Ag, Al, Cd, Yb, Ce, La, Pr, Pu, Sm, Th, Nd, Hf, Zr, Sn, Au, Mn, In, Sr, Ba, U, Ti
Zn	Ni, Hf, Nb, Ta, Ca, Mg, Sc, Sr, Ti
Ga	Fe, Eu, Mg, Mn, Mo, Nb, Sc, Ta
Ge	Mn
Rb	Hg
Sr	Cu, In, Mg, Ni, Rh, Zn
Y	Mg, Mn, Os, Re, Ru, Tc, Ni
Zr	Al, Cr, Cu, Fe, Mn, Ni, Os, Re, Ru, Tc, V, Co, Ir, Pt, Rh, Au, Sn
Nb	Al, Co, Cr, Fe, Ga, Au, Ni, Zn
Mo	Fe, Ga
Tc	Dy, Er, Gd, Hf, Ho, Tc, Tb, Th, Tm, Y, Zr,
Ru	Mg, Dy, Er, Ho, Lu, Nd, Sm, Tb, Tm, Yb, Sc, Zr, Ce, Y
Rh	Al, Cd, Dy, Er, Gd, Hf, Ho, In, Sr, Tm, Zr
Pd	Cd, Gd, Hf, Mg, Sc
Ag	Ca, K. Yb, Ce, Cu
Cd	Ca, Yb, Rh, Ni, Pd, Ir, Pt, Cu, Dy, Gd, Ho
In	Cu, Dy, Er, Gd, Ho, Rh, Ir, Th, U, Sr, Mn, Na, Tb, Tm
Sn	Cu, Fe, Ce, Th, Zr
Cs	Pb, Na
Ba	Cu, Mg, Na, Ni
La	Cu, Os
Ce	Ag, Au, Cu, Mg, Ru, Sn
Pr	Cu, Mn, Ni, Os, Re
Nd	Cu, Mn, Ni, Os, Re, Ru
Sm	Cu, Mn, Ni, Os, Re, Ru,
Eu	Fe, Ga, Mg, Ni, Re
Gd	Cd, In, Rh, Ni, Pd, Ir, Pt, Mn, Os, Re, Tc
Tb	Fe, Mg, Mn, Ni, Os, Re, Ru, In, Ir, Tc
Dy	Cd, In, Rh, Mg, Mn, Ni, Os, Re, Ru, Tc
Ho	Fe, Cd, In, Rh, Ir, Mg, Mn, Ni, Os, Re, Ru, Tc
Er	Al, In, Rh, Ir, Fe, Mg, Mn, Ni, Os, Re, Ru, Tc
Tm	Mg, Mn, Ni, Os, Re, Ru, Tc, In, Rh,
Yb	Cd, Cu, Fe, Mg, Mn, Os, Ru, Ag
Lu	Al, Fe, Mg, Mn, Os, Ru
Hf	Al, Co, Cr, Cu, Fe, Ir, Mn, Os, Pd, Pt, Rh, Au, Re, Tc, V, Zn
Ta	Co, Cr, Fe, Mn, Ga, Au, Zn
W	Fe, Re

Table S7 continuation

Re	Dy, Er, Eu, Gd, Hf, Ho, Nd, Np, Pr, Pu, Sm, Tb, Th, Tm, U, W, Y, Sc, Zr
Os	Am, Dy, Er, Gd, Hf, Ho, La, Lu, Nd, Tb, Tm, U, Yb, Pr, Pu, Sc, Sm, Zr, Y
Ir	Cd, Er, Gd, Hf, Ho, In, Mg, Mn, Sc, Tb, Zr
Pt	Cd, Gd, Hf, Mg, Ca, Zr
Au	Al, K, Ce, Cu, Hf, Na, Nb, Ta, Zr
Hg	K, Rb
Pb	Cs, K
Th	Cu, In, Mg, Mn, Re, Sm, Tc
U	Al, Co, Cu, Fe, In, Mn, Ni, Os, Re
Pu	Cu, Os, Re
Am	Os

Table S8. Distribution of local binding of Bergman and Bergman-based clusters

Formula		Underlying net	Topological types	Number of structures	Formula		Underlying net	Topological types	Number of structures
$1@ico@D32^{8+6}_{f_3^6+f_3^2}$		**bcu-x**	$K_{1.5}Na_{.396}Tl_6Cd_{.3137}$, Rb_3Hg_{20}	**10**	$1@ico@D32^{8}_{b^1}$		**bcu**	$Ho_{16}Mg_{24}Zn_{122}$, $K_{29}NaHg_{48}$ $Mg_{32}(Ag_{13}Al_{36})$	**15**
$1@ico@D32^{6+2+6}_{f_3^2+f_3^6+e^1}$		**bcu-x**	Cr_5Al_8	**16**	$1@ico@D32^{6}_{f_3^2}$		**pcu**	$Na_2Au_6In_5$	**14**
$1@ico@D32^{12}_{v^1}$		**fcu**	$Cu_{12}K_{12}Sn_{21}$	**2**	$1@ico@D32^{6+2}_{f_3^2+f_3^5}$		**hex**	$Sm_{12}Fe_{14}Al_5$	**1**
$1@ico@D32^{12}_{f_3^2}$		**fcu**	$Na_3K_8Tl1_3$	**1**	$1@ico@D32_{mol}$		Isolated**	$Li_{33.3}Ba_{13.08}Ca_{2.96}$	**2**
$1@ico@D32^{4+4+4}_{f_3^2+b^1+b^2}$		**gsp1**	$Li_5Ca_{18}In_{25.07}$	**1**	$1@ico@D32@D98^{12}_{e^1}$		**fcu**	$Li_{33.3}Ba_{13.08}Ca_{2.96}$	**2**
$0@ico@D32^{2+8}_{f_8^2+b^{10}}$		**bct**	$Na_{10}Ga_6Sn_3$	**1**	$0@ico@D32@D80^{4+2}_{b^{40}+v^2}$		**hxl***	$Na_{128}Au_{81}Ga_{275}$,	**1**
$0@ico@D32^{8}_{b^1}$		**bcu**	$K_{49}Tl_{108}$, $K_3Na_{26}In_{48}$, $Al_{88.7}Cu_{19.3}Li_{52}$, $Ga_{22.13}Li_{11.33}Zn_{2.66}$,	**36**	$0@ico@D32@D86^{6}_{v^1+e^4}$		**pcu**	$K_{49}Tl_{108}$	**1**
$0@ico@D32^{6}_{b^2}$		**hxl***	Na_7Ga_{13}	**1**	$0@ico@D32@D92^{6}_{v^1+e^4}$		**pcu**	$K_{49}Tl_{108}$	**1**
$0@ico@D32^{2}_{b^1}$		chain*	$Na_{16}Zn_{13.54}Sn_{13.46}$	**1**	$0@ico@D32@D102^{8+6}_{f_3^{14}+f_3^2}$		**bcu-x**	$CaCd_6$	**17**
$0@ico@D32_{mol}$		Isolated**	$Ga_{19.56}Li_3Na_5$, $K_{34}In_{89.95}Zn_{13.05}$, $(Cu_6Ga_{46.5})Na_{17}$, $Au_{115.29}Ca_{24}Sn_{34.81}$, $CaCd_6$, $K_{34}In_{91.05}Mg_{13.95}$, $K_{39}In_{80}$, $K_{14}Na_{21}Cd_{17}Ga_{82}$, $Na_{128}Au_{81}Ga_{275}$	**36**	$0@ico@D32@D110^{8+6}_{f_3^{14}+f_3^2}$		**bcu-x**	$Au_{115.29}Ca_{24}Sn_{34.81}$	**1**
$0@ico@D32@D80^{6+6}_{b^{40}+}$		**fcu**	$(Cu_6Ga_{46.5})Na_{17}$, $K_{14}Na_{21}Cd_{17}Ga_{82}$, $K_{34}In_{89.95}Zn_{13.05}$, $K_{34}In_{91.05}Mg_{13.95}$	**15**	$0@ico@D32@D98^{6}_{f_3^6}$		**hxl***	$K_{39}In_{80}$, $K_{34}In_{89.95}Zn_{13.05}$	**5**
					$0@ico@D32@D80^{6}_{b^{40}}$		**hxl***	$(Cu_6Ga_{46.5})Na_{17}$	**9**

* – ignoring bonds between icosahedra that unite layers into a 3D framework; ** - all contacts of the nanocluster are with nanoclusters of other type.

Table S9. Correlations between the underlying net topology and the crystal system

Underlying net topology	Crystal System	Number of structures
bcu-x	Cubic	435
	Tetragonal	3
fcu	Tetragonal	1
	Trigonal	2
	Hexagonal	1
	Orthorhombic	1
	Cubic	9
tca	Hexagonal	81
ncb	Cubic	22
hex	Hexagonal	771
	Orthorhombic	38
	Monoclinic	5
	Trigonal	2
$(3^6.4^{12}.5^3)$	Orthorhombic	2
crs	Cubic	100
pcu	Cubic	19
hxl	Orthorhombic	3
	Monoclinic	3
	Trigonal	1
dia	Orthorhombic	5
sql	Orthorhombic	1
lcy	Cubic	1

Table S10. Correlations between the crystal system and the underlying net topology

Crystal System	Underlying net topology	Number of structures
Cubic	**bcu-x**	435
	crs	100
	ncb	22
	pcu	19
	fcu	9
	lcy	1
Hexagonal	**hex**	771
	tca	81
	fcu	1
Trigonal	**fcu**	2
	hex	2
	hxl	1
Tetragonal	**bcu-x**	3
	fcu	1
Orthorhombic	**hex**	38
	dia	5
	hxl	3
	$(\mathbf{3^6.4^{12}.5^3})$	2
	fcu	1
	sql	1
Monoclinic	**hex**	5
	hxl	3